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Threshold energy and impact ionization scattering rate calculations for strained silicon

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Abstract In this work, a comprehensive method to obtain the impact ionization rate has been developed and applied to both strained and unstrained silicon. Special care was taken to find criteria which support the appropriateness of our choice of numerical methods, especially the integration method and the delta distribution approximation. The algorithm developed takes into account both efficiency and accuracy requirements. We investigate the impact of introducing stress on the impact ionization rate and observe that the impact ionization threshold is shifted to lower energies, but by a smaller amount than the band gap is lowered. This can be explained by the availability of fewer possibilities to satisfy both energy and momentum conservation conditions at the same time.

Keywords Impact ionization · Strained silicon · TCAD

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1 Introduction

Impact ionization is an important scattering process in semiconductors where a high–energetic particle creates an electron–hole pair. This concerns e.g. device reliability where the substrate current in MOSFETs serves as a monitor for hot electrons, which are responsible for oxide degradation, or avalanche breakdown which destroys the device. More recently, it is also relevant for the operation of partially–depleted silicon-on-insulator (PD–SOI) MOSFETs where the generated holes give rise to the floating-body effect (cf. [1, 2]). On the other hand, strained silicon has now become indispensable for further performance improvement of CMOS technology. From a simulation viewpoint, this requires knowledge of the stress–dependence of all transport parameters. While impact ionization has already been studied extensively in unstrained silicon (e.g. [3, 4]), transport parameter calculations for strained Si have so far been restricted to drift velocity and mobility (e.g. [5]). It is therefore the main aim of this paper to compute the impact ionization rates in silicon under biaxial tensile strain. In particular, this includes the (to our knowledge) first direct extraction of the impact ionization threshold energies from energy and momentum conservation in the corresponding full–band structures. In addition, our investigation also includes an optimized version of the Monte Carlo integration of scattering rates which is verified for the random-**k** approximation where the exact result is available in terms of the density-of-states.

2 Numerical methodology

We have devised an algorithm that obtains the threshold energies of impact ionization by means of numerical optimiza-

tion based on the downhill simplex method by Nelder and Mead [6]. It only uses full-band structure information as input data and obtains the respective threshold energies and a list of possible processes based on energy and momentum conservation. Results of the threshold determination are used as a starting point for the impact ionization rate integration.

In performing the so-called random-**k** approximation, neglecting momentum conservation yields the (hole-initiated) impact ionization rate

$$S_{II}^{rk}(v,\mathbf{k_v}) = \frac{2\pi}{\hbar}\tilde{M}^2 \sum_{\substack{c',v'\\ v''\geq v'}} \sum_{\mathbf{k}_{v'}} \sum_{\mathbf{k}_{c'}} \sum_{\mathbf{k}_{v''}} \frac{1}{N}\delta(\Delta\epsilon), \tag{1}$$

where

$$\Delta\epsilon = E_v(\mathbf{k_v}) - E_{v'}(\mathbf{k_{v'}}) - E_{v''}(\mathbf{k_{v''}}) - E_{c'}(\mathbf{k_{c'}}) - E_g \tag{2}$$

characterizes the energy conservation. E_g and N denote the band gap and number of unit cells considered.

Since this nine-dimensional integral is also known in terms of the density of states

$$\begin{aligned} S_{II}^{rk}(E_v(v,\mathbf{k_v})) = s_0^{rk} \sum_{\substack{c',v'\\ v''\geq v'}} \int_0^{\hat{E}'_{v'}} dE'_{v'} \int_0^{\hat{E}'_{c'}} dE'_{c'} \\ \times \mathcal{D}_{c'}(E'_{c'})\mathcal{D}_{v'}(E'_{v'})\mathcal{D}_{v''}(E_v(\mathbf{k_v}) \\ -E'_{v'} - E'_{c'} - E_g), \end{aligned} \tag{3}$$

it can be used as a test case for impact ionization rate integration approaches. Both the integration method and delta distribution approximation applied to Eq. (1) have been optimized to yield results as close to the ones obtained from expression (3) as possible. We then evaluate the momentum conserving impact ionization rate

$$S_{II}(v,\mathbf{k_v}) = s_o \sum_{\substack{v'\\ v''\geq v'\\ c'}} \sum_{\mathbf{k}_{v'}} \sum_{\mathbf{k}_{c'}} \sum_{\mathbf{k}_{v''}} \delta_{\mathbf{k}_v,\mathbf{k}_{v'}+\mathbf{k}_{v''}+\mathbf{k}_{c'}}\delta(\Delta\epsilon). \tag{4}$$

$\Delta\epsilon$ here is defined as in Eq. (2). The factor s_0 reads

$$s_0 = \frac{2\pi}{\hbar}\tilde{M}^2, \tag{5}$$

where the matrix element $\tilde{M}$ will be replaced by a dimensionless matrix element $\bar{M}$ using

$$\tilde{M} = \bar{M}\frac{e^2}{\Omega\epsilon_0}\left(\frac{a_0}{2\pi}\right)^2. \tag{6}$$

Table 1 Optimized parameter set for the modified Lorentz profile

cutoff δ (eV)	half-width η (eV)
0.25	0.15

In Eq. (6), Ω and a_0 denote the unit cell volume and lattice constant respectively. Note that we use a constant matrix element, which either comes from the derivation of the Boltzmann equation based on localized Wannier functions [8] or by approximating the matrix element resulting from pseudo–Bloch functions as constant [4].

For the impact ionization rate integration, we have obtained the best results using a modified Lorentz profile with optimized cutoff and half-width parameters serving as a delta distribution approximation and a Monte-Carlo integration algorithm with stratified sampling and importance sampling (cf. [7]). The shape of our delta distribution approximation is given by

$$\delta(x) = \begin{cases} \dfrac{1}{2\arctan\left(\dfrac{\delta}{2\eta}\right)} \dfrac{\eta}{|x|^2+\eta^2} & |x| \leq \delta/2 \\ 0 & \text{elsewhere,} \end{cases} \tag{7}$$

and yields more accurate results than simple box approximations (e.g. [9]). The optimized parameter set can be read off from Table 1.

Furthermore, we optimized our Monte Carlo integration algorithm and compared it to equidistant point integration methods (e.g. [10]). Some of the comparisons of different delta distribution approximations and integration methods are illustrated in Fig. 1.

Then, we evaluate the momentum conserving impact ionization rate in its energy-averaged form

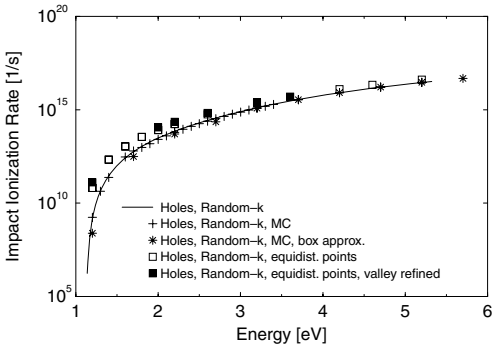

Fig. 1 Delta distribution and integration method comparison for the random–**k** method. Our results are marked with +. Stars denote results of approximating the delta function by a box. Open and closed square boxes denote equidistant integration point methods without and with refinement in the valleys, respectively

Table 2 Fitting parameters for the electron impact ionization rate in Si

j	$E_{th,j}$ (eV)	P_j (s^{-1})	a_j
1	1.13	$2.0 \cdot 10^{12}$	2.981
2	1.6	$2.3 \cdot 10^{14}$	2.978
3	2.6	$1.8 \cdot 10^{16}$	2.490

Table 3 Fitting parameters for the hole impact ionization rate in Si

j	$E_{th,j}$ (eV)	$P_j(s^{-1})$	a_j
1	1.33	$6.58 \cdot 10^{13}$	4.172

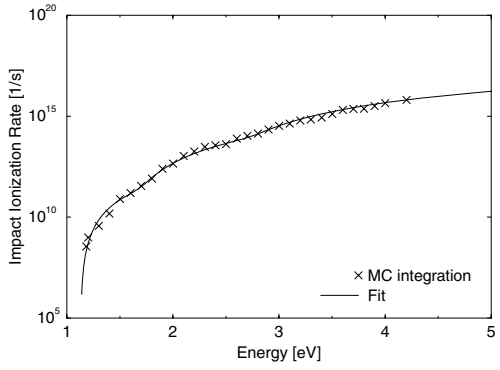

Fig. 2 Electron initiated impact ionization rate in Si

$$R(E) = \frac{\sum_v \int d^3\mathbf{k_v}\delta(E - E_v(\mathbf{k_v}))S_{II}(v, \mathbf{k_v})}{\sum_v \int d^3\mathbf{k_v}\delta(E - E_v(\mathbf{k_v}))} \tag{8}$$

and fit the results to a generalized multi-component Keldysh formula

$$S(E) = \sum_{j=1}^{n} \Theta(E - E_{th,j})\, P_j \left(\frac{E - E_{th,j}}{E_{th,j}}\right)^{a_j} \tag{9}$$

(in the original Keldysh formula, n was set equal to one). The results for electron initiated impact ionization are plotted in Fig. 2; numerical values of the fitting parameters are given in Table 2.

For the hole initiated impact ionization rate, a one component-formula of type (9) turns out to be sufficient. The values obtained from our least square fit are given in Table 3.

We observe that steep steps in the electron-initiated impact ionization rate are due to the number of allowed processes times the density of states (cf. Fig. 3 and Table 2). In our calculations, the dimensionless matrix element $\bar{M}$ has been set to unity. By fitting our results to experimental impact ionization coefficient values obtained by [11] and [12], we get e.g. $\bar{M}^2 = 0.14$ for electron–initiated impact ionization in unstrained Si.

Table 4 Threshold energies for electron and hole initiated impact ionization in silicon under biaxial tensile strain with different substrate germanium content

Ge content [%]	Band gap (eV)	$E_{th}^{(e^-)}$ (eV)	$E_{th}^{(h^+)}$ (eV)
0	1.12	1.140	1.367
10	1.063	1.091	1.337
20	1.003	1.036	1.314

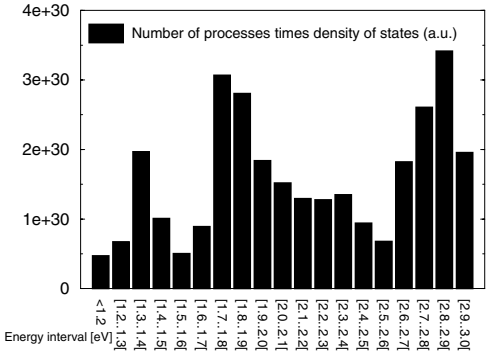

Fig. 3 Density of states times number of processes (a. u.) starting to be accessible per energy interval in eV for electron initiated impact ionization in Si

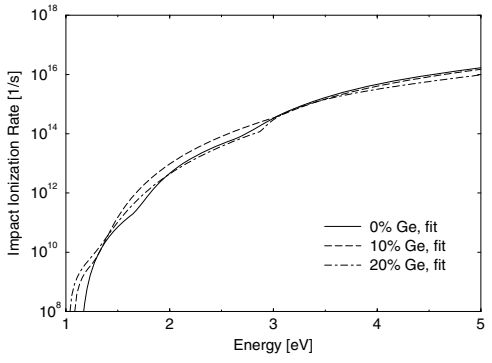

Fig. 4 Electron initiated impact ionization rates in strained silicon

3 Results for strained Si

Under biaxial tensile stress, the silicon band structure is being changed, where in particular the band gap is reduced. Results of the threshold determination for strained Si are presented in Table 4.We observe that the threshold energy is lowered with increasing Ge content by a smaller amount than the band gap is reduced, which can be explained by the availability of fewer possibilites to fulfill both momentum and energy conservation simultaneously.

Figures 4 and 5 show the results for Si under biaxial tensile strain with different Ge substrate contents for electron and hole initiated impact ionization.

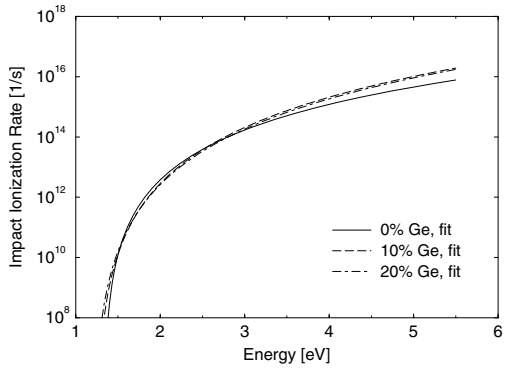

Fig. 5 Hole initiated impact ionization rates in strained silicon

4 Conclusion

We have presented a new comprehensive method for the calculation of impact ionization scattering rates, which can be applied to any semiconductor, especially also to uniaxially-stressed Si. Thus, a sound basis has been given for the inclusion of impact ionization in the simulation especially of strained-Si devices.

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References

1. Shahidi, G.G.: SOI technology for the GHz era, IBM J. Res. & Dev. **46** (2/3), 121 (2002)
2. Rafi, J.M., Simoen, E., Mercha, A., Campabadal, F.: Impact of hot-carrier stress on gate-induced floating body effects and drain current transients of thin gate oxide partially depleted SOI nMOSFETs, Claeys, C. Solid-State Electr. **49**, 1536 (2005)
3. Cartier, E., Fischetti, M.V., Eklund, E.A., McFeely, F.R.: Impact ionization in silicon. Appl. Phys. Lett. **62**, 3339 (1993)
4. Fischetti, M.V., Sano, N., Laux, S.E., Natori, K.: Full-band-structure theory of high-field transport and impact ionization of electrons and holes in Ge, Si, and GaAs. IEEE J. TCAD **3** (1997)
5. Bufler, F.M.: Full-band Monte Carlo simulation of electrons and holes in strained Si and SiGe, Herbert Utz Verlag (1998)
6. Nelder, J.A., Mead, R.: A simplex method for function minimization, The Comput. J. **7**(4), 308 (1965)
7. Hammersley, J.M., Handscomb, D.C.: Monte Carlo methods, London: Methuen (1975)
8. Bufler, F.M.: Decomposition of the Coulomb interaction into self–consistent fields and local scattering terms, J. Phys. Condens. Matter **9**, 3741 (1997)
9. Sano, N., Yoshii, A.: Impact-ionization theory consistent with a realistic band structure of silicon. Phys. Rev. B **45**, 4171 (1992)
10. Reigrotzki, M.: Theoretische Untersuchungen zur Stossionisation und zum Hochfeldtransport in Halbleitern, doctoral thesis, Universität Rostock, Rostock (1998)
11. Robbins, V.M., Wang, T., Brennan, K.F., Hess, K., Stillman, G.E.: Electron and hole impact ionization coefficients in (100) and in (111) Si, J. Appl. Phys. **58**, 4614 (1985)
12. Takayanagi, I., Matsumoto, K. Nakamura. J.: Measurement of electron impact ionization coefficient in bulk silicon under a low electric field. J. Appl. Phys. **72**, 1989 (1992)